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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
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NEWS 3 May 10 PROUSDDR now available on STN
NEWS 4 May 19 PROUSDDR: One FREE connect hour, per account, in both May
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SDIs in CAplus
NEWS 9 May 27 CAplus super roles and document types searchable in REGISTRY
NEWS 10 May 27 Explore APOLLIT with free connect time in June 2004
NEWS 11 Jun 22 STN Patent Forums to be held July 19-22, 2004
NEWS 12 Jun 28 Additional enzyme-catalyzed reactions added to CASREACT
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NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:42:57 ON 01 JUL 2004

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CAPLUS' ENTERED AT 09:43:13 ON 01 JUL 2004

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FILE COVERS 1907 - 1 Jul 2004 VOL 141 ISS 1
FILE LAST UPDATED: 30 Jun 2004 (20040630/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> esterif?

L1 121483 ESTERIF?

=> acetl chloride

2 ACETL

1 ACETLS

3 ACETL

(ACETL OR ACETLS)

992807 CHLORIDE

148850 CHLORIDES

1060604 CHLORIDE

(CHLORIDE OR CHLORIDES)

L2 0 ACETL CHLORIDE

(ACETL(W)CHLORIDE)

=> acetyl chloride

142650 ACETYL

62 ACETYLS

142685 ACETYL

(ACETYL OR ACETYLS)

992807 CHLORIDE

148850 CHLORIDES

1060604 CHLORIDE

(CHLORIDE OR CHLORIDES)

L3 10351 ACETYL CHLORIDE

(ACETYL(W)CHLORIDE)

=> cataly?

L4 1195325 CATALY?

=> 13(1)14

L5 671 L3(L)L4

=> 11 and 15

L6 39 L1 AND L5

=> d 16 29-39 ti

L6 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI 2,4-Dinitro-6-sec-butylphenyl acetate

L6 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI Racemization of phenanthrene 3,4-oxide. Absolute stereochemistry of cis-

and trans-phenanthrene 3,4-dihydrodiols

L6 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI Trichloroacetyl chloride

L6 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI Determination of the composition of aliphatic acids in food products

L6 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI Poly(oxymethylenes)

L6 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI Polymerization catalyst for trioxane

L6 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI New **esterification** procedures in peptide chemistry. I. Selective **esterification** with new catalysts

L6 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI Amino yarns

L6 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI **Esterification** of unstable alcohols

L6 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI **Esterification** of proteins by alcohols of low molecular weight

L6 ANSWER 39 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI Ester formation under the catalytic influence of acid chlorides

=> d 16 35,37,38 ti fbib abs

L6 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
TI New **esterification** procedures in peptide chemistry. I. Selective **esterification** with new catalysts
AN 1961:75814 CAPLUS
DN 55:75814
OREF 55:14318d-f
TI New **esterification** procedures in peptide chemistry. I. Selective **esterification** with new catalysts
AU Taschner, Emil; Wasielewski, Czeslaw
CS Tech. Hochschule Danzig, Pol.
SO Ann. (1961), 640, 136-9
DT Journal
LA Unavailable
AB The **esterification** of 1 millimole phthaloylglycine in 2 ml. MeOH at 20° 48 hrs. in the presence of 0.01 millimole of the following catalysts gave the following yields: AsCl₃ (93%), PCl₅ (91%), PBr₅ (82%), SO₂Cl₂ (91%), SOCl₂ (82%), SiCl₄ (87%), AcCl (82%), POCl₃ (77%), PCl₃ (68%), AlCl₃ (69%), POBr₃ (68%), ClSO₃H (59%), H₂SO₄ (55%), PhSO₂Cl (50%), MeSO₂Cl (46%), p-MeC₆H₄SO₂Cl (37%), HCl (36%), SnCl₄ (32%), SbCl₃ (30%), HBr (18%), ZnCl₂ (0%). The following compds. were prepared by the use of SO₂Cl₂: phthaloylglycine Me ester, m. 116°, 91% yield; tosylglycine Me ester, m. 91-3°, 94%; phthaloyl-DL-leucine Me ester, m. 81°, 90%; phthaloyl-DL-valine Me ester, m. 39-41°, 94%; dibenzoyl-L-tyrosine Me ester, m. 144°, 93%; carbobenzoxy-L-asparagine Me ester, m. 143-7°, 86%; tosyl-L-asparagine Me ester, m. 181°, 91%; tosyl-L-glutamine Me ester, oil; tosyl-L-pyroglutamic acid, m. 122°, 48%; phthaloylglycyl-DL-valine Me ester, m. 196°, 91%; phthaloylglycyl-DL-asparagine Me ester, m. 223°, 90%; carbobenzoxy-DL-leucylglycine Me ester, m. 76°, 90%.

L6 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
 TI **Esterification** of unstable alcohols
 AN 1952:48293 CAPLUS
 DN 46:48293
 OREF 46:7991g-h
 TI **Esterification** of unstable alcohols
 AU Mills, J. A.
 CS Univ. Adelaide, Australia
 SO Journal of the Chemical Society, Abstracts (1951) 2332-4
 CODEN: JCSAAZ; ISSN: 0590-9791
 DT Journal
 LA Unavailable
 OS CASREACT 46:48293
 AB Poor yields of esters from the reaction of certain alcs. with acid chlorides in C₅H₅N are probably due to decomposition **catalyzed** by the pyridinium ion. Good yields may be obtained by avoiding an excess of C₅H₅N and working in a solvent which precipitated C₅H₅N.HCl as it is formed. Me₂C:CHCH(OH)Me [0.02 mol. C₅H₅N in 40 ml. petr. ether (b. 60-90°)], treated with 0.2 mol. of the acid chloride, kept overnight in the refrigerator, and the filtrate washed with 1% aqueous Na₂CO₃ and H₂O, give about 80% of the esters: p-nitrobenzoate, m. 71-2°; p-nitrophenoxycetate, pale yellow, m. 90-1°; (p-phenylazophenoxy)acetate, pale yellow, m. 59-60°. These esters decompose suddenly between 110 and 150°. (p-Phenylazophenoxy) **acetyl chloride**, orange, m. 88-90°.

L6 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2004 ACS on STN
 TI **Esterification** of proteins by alcohols of low molecular weight
 AN 1946:6744 CAPLUS
 DN 40:6744
 OREF 40:1166b-f
 TI **Esterification** of proteins by alcohols of low molecular weight
 AU Fraenkel-Conrat, Heinz L.; Olcott, Harold S.
 CS Western Regional Research Lab., Albany, CA
 SO Journal of Biological Chemistry (1945), 161, 259-68
 CODEN: JBCHA3; ISSN: 0021-9258
 DT Journal
 LA Unavailable
 AB The reaction of Freudenberg and Jacob (C.A. 35,7371.7) whereby acids are **esterified** by the action of alcs. in the presence of acid chlorides has been applied to proteins. Polyglutamic acid with MeOH in 100-fold excess, 0.5 N with respect to HCl or AcCl, at 22-4° was 97% **esterified** in 1 day, with solution soon after the reaction began. Under similar conditions, EtOH gave 54% in 1 day, 83% in 6 days; iso-PrOH 0 and 4%; PhCH₂OH, -, 6%; HO(CH₂)₃OH 40, 76%, resp. Proteins which gave similar results were bovine serum albumin (I), β-lactoglobulin (II), insulin (III), lysozyme (IV), and the pituitary adrenocorticotrophic (V) and lactogenic (VI) hormones. The clear alc. solns. became more viscous and set to gels after 24 hrs. Addition of Et₂O converted the gel to white powders soluble in H₂O and dilute salt solns. They were precipitated from these solns. at pH 7-8 and did not redissolve at pH 10-11. Egg albumin (VII) dissolved only in HO(CH₂)₃OH and gave gels without passing into complete solution. Other proteins studied, although some appeared unaltered, took up variable amts. of MeOH. The ratio of MeO introduced to the original CO₂H for II was 13.6:13.7; I, 10.3:10.8; casein, 10.0:16.0; VII, 9.0: 9.5; III, 8.4:8.0; VI, 7.9:8.8; hoof powder, 6.2:6.6; IV, 4.2:?.; gluten, 3.6:3.6; silk fibroin, 2.3:2.4; gliadin, 2.1:3.9; deamidated gluten, 18.2:?. With alcs. other than MeOH the reaction was much less complete. Contrary to F. and J., HCl and AcCl were equally good catalysts for the reaction when used in 30-50 equivs. of catalyst per 104 g. of protein, and for the **esterification** of such simple acids as stearic, acetic, lactic,

galacturonic, benzoyl-dl-alanine, acetyl-dl-tryptophan, and N-benzoyl-dl-serine. Thio-glycolic and BzOH were **esterified** very slowly under these conditions (6% in 24 hrs.). Limitations of the dye techniques for the determination of acid and basic groups in proteins are discussed.

=> creatine

25414 CREATINE
26 CREATINES
L7 25419 CREATINE
(CREATINE OR CREATINES)

=> d his

(FILE 'HOME' ENTERED AT 09:42:57 ON 01 JUL 2004)

FILE 'CAPLUS' ENTERED AT 09:43:13 ON 01 JUL 2004

L1 121483 ESTERIF?
L2 0 ACETL CHLORIDE
L3 10351 ACETYL CHLORIDE
L4 1195325 CATALY?
L5 671 L3(L)L4
L6 39 L1 AND L5
L7 25419 CREATINE

=> 16 and 17

L8 0 L6 AND L7

=> 15 and 17

L9 0 L5 AND L7

=> unstable

90186 UNSTABLE
3 UNSTABLES
L10 90188 UNSTABLE
(UNSTABLE OR UNSTABLES)

=> 17 and 110

L11 164 L7 AND L10

=> d 111 154-164 ti

L11 ANSWER 154 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Chemical composition and enzymes of the smooth muscle

L11 ANSWER 155 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Stability of thiamine solution. I. Influence of protein compounds and blood plasma on the stability of thiamine or cocarboxylase solution

L11 ANSWER 156 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI The mechanism of acid secretion by gastric mucosa. II. An extended theory

L11 ANSWER 157 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI The use of sodium sulfate for the preparation of concentrated protein-free tissue extracts

L11 ANSWER 158 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Isolation of chemically **unstable** substances from animal tissues

L11 ANSWER 159 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI **Creatine** and creatinine. II. Alleged acyl derivatives of **creatine**

L11 ANSWER 160 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI A possible new factor in the chemical mechanism of muscular contraction

L11 ANSWER 161 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Water-soluble vitamin and bacterial growth

L11 ANSWER 162 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Water-soluble vitamin and bacterial growth

L11 ANSWER 163 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Blood analyses in cases of catatonic dementia precoc

L11 ANSWER 164 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Disodiumphenolphthaleinquinone or Disodium-aci-phenolphthalein

=> d l11 158,159 ti

L11 ANSWER 158 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Isolation of chemically **unstable** substances from animal tissues

L11 ANSWER 159 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI **Creatine** and creatinine. II. Alleged acyl derivatives of
creatine

=> d l11 158,159 ti fbib abs

L11 ANSWER 158 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI Isolation of chemically **unstable** substances from animal tissues
AN 1932:54309 CAPLUS
DN 26:54309
OREF 26:5591i
TI Isolation of chemically **unstable** substances from animal tissues
AU Eggleton, M. G.; Eggleton, P.
SO Nature (London, United Kingdom) (1932), 130, 275
CODEN: NATUAS; ISSN: 0028-0836
DT Journal
LA Unavailable
AB Minced muscle is mixed with 40% of its weight of anhydrous Na2SO4 and the expressed H2O separated at 32°. When cooled to 0°, 96% of the Na2SO4 crystallizes out, leaving a protein-free highly concentrated extract
This technic has been applied to the isolation of **creatine**, carnosine and anserine.

L11 ANSWER 159 OF 164 CAPLUS COPYRIGHT 2004 ACS on STN
TI **Creatine** and creatinine. II. Alleged acyl derivatives of
creatine
AN 1932:54033 CAPLUS
DN 26:54033
OREF 26:5548e-f
TI **Creatine** and creatinine. II. Alleged acyl derivatives of
creatine
AU Ing, H. R.
SO Journal of the Chemical Society, Abstracts (1932) 2198-200
CODEN: JCSAAZ; ISSN: 0590-9791
DT Journal
LA Unavailable
AB cf. C. A. 26, 5076. The "diacetylcreatine" of Erlenmeyer (Ann. 284, 49(1895)) is sym-(N-acetylsarcosyl)acetylurea, AcMeNCH2CONH-CONHAc (I); the only other product formed in the acetylation is 1-methylhydantoin.

The structure of I was established by its reaction with NH₃, the products being AcNH-CONH₂ and N-acetylsarcosine amide, m. 140-1°, also prepared from sarcosine through the Me ester of the Ac derivative. It is assumed

that the Ac₂O attacks the tert-N atom of **creatine**, an **unstable** quaternary salt being formed, which isomerizes to an imino acid anhydride, AcMeNCH₂CONHC(OAc):NH; migration of Ac from O to N gives I. The "phthalylidicreatine" of Urano (C. A. 1, 876) is shown to be dicreatinine phthalate, m. 223° (decomposition).

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

47.50

47.71

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-3.68

-3.68

FILE 'REGISTRY' ENTERED AT 09:57:24 ON 01 JUL 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JUN 2004 HIGHEST RN 701907-96-2

DICTIONARY FILE UPDATES: 30 JUN 2004 HIGHEST RN 701907-96-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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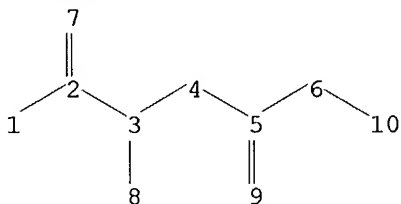
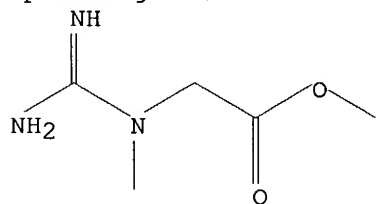
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Examination Auxillary files\10647825\10647825 creatine prod.str



chain nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-2 2-3 2-7 3-4 3-8 4-5 5-6 5-9 6-10

exact/norm bonds :

1-2 2-3 2-7 3-4 3-8 5-6 5-9 6-10

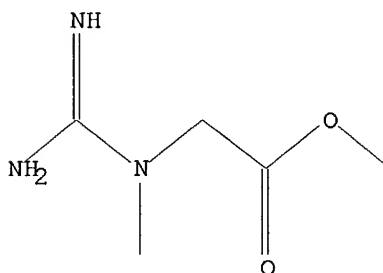
exact bonds :

4-5

Hydrogen count :
4:>= minimum 2 8:>= minimum 3
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L12 STRUCTURE UPLOADED

=> d 112
L12 HAS NO ANSWERS
L12 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 112 sss sam
SAMPLE SEARCH INITIATED 09:57:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 10 TO ITERATE

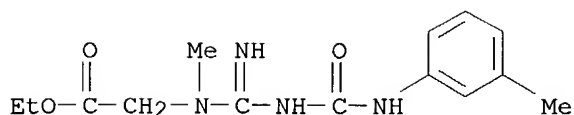
100.0% PROCESSED 10 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 11 TO 389
PROJECTED ANSWERS: 1 TO 80

L13 1 SEA SSS SAM L12

=> d 113

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 102908-32-7 REGISTRY
CN Glycine, N-[imino[[[(3-methylphenyl)amino]carbonyl]amino]methyl]-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)
MF C14 H20 N4 O3 . Cl H
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)



● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> search l12 sss full
FULL SEARCH INITIATED 09:59:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 242 TO ITERATE

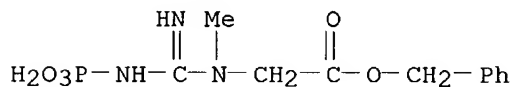
100.0% PROCESSED 242 ITERATIONS
SEARCH TIME: 00.00.01

35 ANSWERS

L14 35 SEA SSS FUL L12

=> d scan

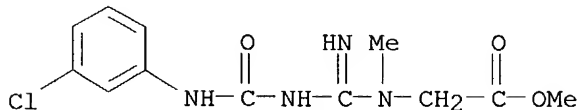
L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Glycine, N-[imino(phosphonoamino)methyl]-N-methyl-, 1-(phenylmethyl)
ester, monosodium salt (9CI)
MF C11 H16 N3 O5 P . Na



● Na

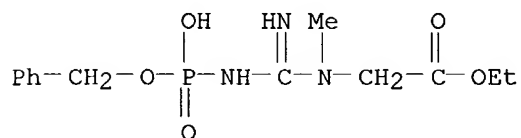
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Glycine, N-[[[(3-chlorophenyl)amino]carbonyl]amino]iminomethyl]-N-methyl-,
methyl ester, monohydrochloride (9CI)
MF C12 H15 Cl N4 O3 . Cl H



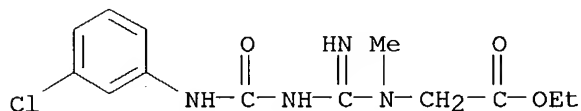
● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2-Oxa-4,6-diaza-3-phosphaoctan-8-oic acid, 3-hydroxy-5-imino-6-methyl-1-phenyl-, ethyl ester, 3-oxide, monosodium salt (9CI)
 MF C13 H20 N3 O5 P . Na



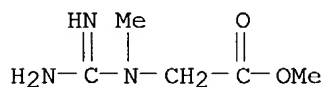
● Na

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[[[(3-chlorophenyl)amino]carbonyl]amino]iminomethyl]-N-methyl-, ethyl ester, monohydrochloride (9CI)
 MF C13 H17 Cl N4 O3 . Cl H



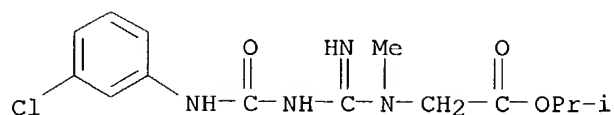
● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-(aminoiminomethyl)-N-methyl-, methyl ester (9CI)
 MF C5 H11 N3 O2
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

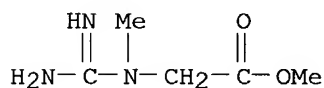
L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[[[(3-chlorophenyl)amino]carbonyl]amino]iminomethyl]-N-methyl-, 1-methylethyl ester, monohydrochloride (9CI)
 MF C14 H19 Cl N4 O3 . Cl H



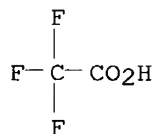
● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-(aminoiminomethyl)-N-methyl-, methyl ester,
 mono(trifluoroacetate) (9CI)
 MF C5 H11 N3 O2 . C2 H F3 O2

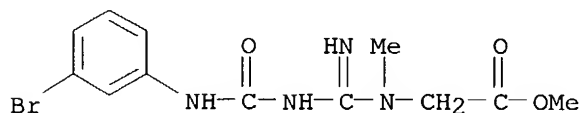
CM 1



CM 2

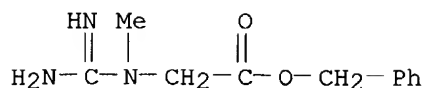


L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[[[(3-bromophenyl)amino]carbonyl]amino]iminomethyl]-N-methyl-,
 methyl ester, monohydrochloride (9CI)
 MF C12 H15 Br N4 O3 . Cl H



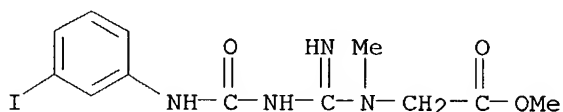
● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-(aminoiminomethyl)-N-methyl-, phenylmethyl ester (9CI)
 MF C11 H15 N3 O2
 CI COM



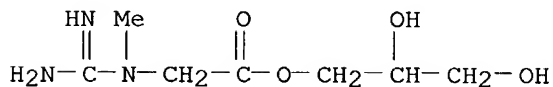
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[imino[[[(3-iodophenyl)amino]carbonyl]amino]methyl]-N-methyl-,
 methyl ester, monohydrochloride (9CI)
 MF C12 H15 I N4 O3 . Cl H



● HCl

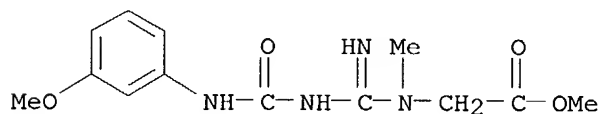
L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-(aminoiminomethyl)-N-methyl-, 2,3-dihydroxypropyl ester (9CI)
 MF C7 H15 N3 O4
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
 HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

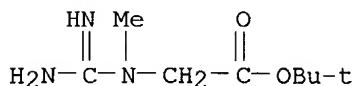
L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[imino[[[(3-methoxyphenyl)amino]carbonyl]amino]methyl]-N-methyl-,
 methyl ester, monohydrochloride (9CI)
 MF C13 H18 N4 O4 . Cl H



● HCl

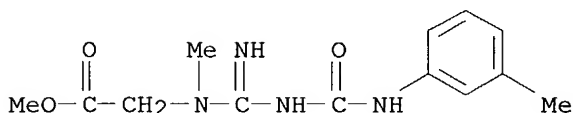
L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Glycine, N-(aminoiminomethyl)-N-methyl-, 1,1-dimethylethyl ester (9CI)
 MF C8 H17 N3 O2
 CI COM



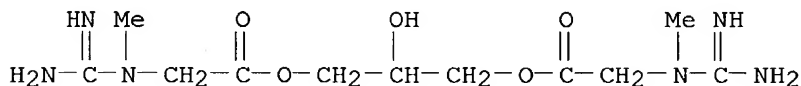
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[imino[[[(3-methylphenyl)amino]carbonyl]amino]methyl]-N-methyl-, methyl ester, monohydrochloride (9CI)
 MF C13 H18 N4 O3 . Cl H



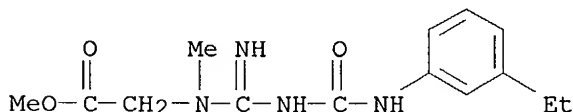
● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-(aminoiminomethyl)-N-methyl-, 2-hydroxy-1,3-propanediyl ester (9CI)
 MF C11 H22 N6 O5
 CI COM



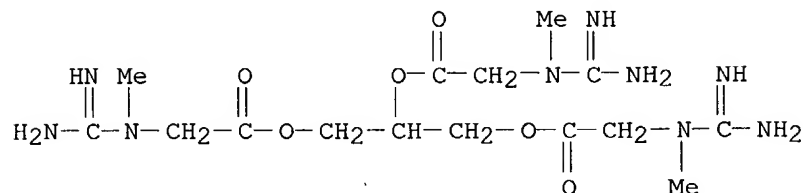
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[[[[(3-ethylphenyl)amino]carbonyl]amino]iminomethyl]-N-methyl-, methyl ester, monohydrochloride (9CI)
 MF C14 H20 N4 O3 . Cl H



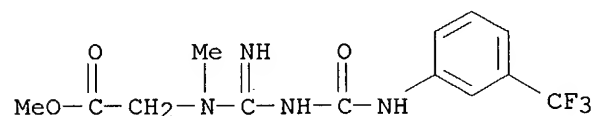
● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-(aminoiminomethyl)-N-methyl-, 1,2,3-propanetriyl ester (9CI)
 MF C15 H29 N9 O6



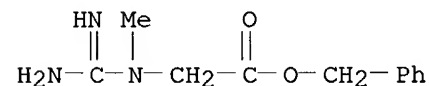
..**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[imino[[[3-(trifluoromethyl)phenyl]amino]carbonyl]amino]methyl
]-N-methyl-, methyl ester, monohydrochloride (9CI)
 MF C13 H15 F3 N4 O3 . Cl H



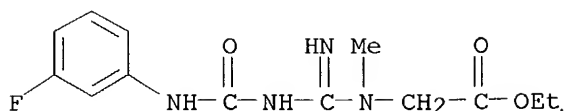
● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-(aminoiminomethyl)-N-methyl-, phenylmethyl ester,
 monohydrochloride (9CI)
 MF C11 H15 N3 O2 . Cl H



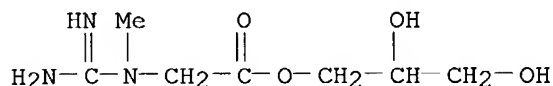
● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[[[[(3-fluorophenyl)amino]carbonyl]amino]iminomethyl]-N-methyl-
 , ethyl ester, monohydrochloride (9CI)
 MF C13 H17 F N4 O3 . Cl H



● HCl

L14 35 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-(aminoiminomethyl)-N-methyl-, 2,3-dihydroxypropyl ester,
 monohydrochloride (9CI)
 MF C7 H15 N3 O4 . Cl H



● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
158.87	206.58

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
0.00	-3.68

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FILE 'CAPLUS' ENTERED AT 10:00:28 ON 01 JUL 2004

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FILE COVERS 1907 - 1 Jul 2004 VOL 141 ISS 1

FILE LAST UPDATED: 30 Jun 2004 (20040630/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 114

L15 12 L14

=> d l15 1-12 ti

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Methods of treating cognitive dysfunction by modulating brain energy metabolism by using an effective amount of a creatine compound-protein conjugate

L15 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Creatine ester pronutrient compounds and formulations

L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI A Novel Traceless Resin-Bound Guanidinyllating Reagent for Secondary Amines To Prepare N,N-Disubstituted Guanidines

L15 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Preparation of phosphocreatine derivatives

L15 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Inhibitory effects of O-benzyl-phosphocreatine ethyl ester in rabbit myocardium

L15 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Electrophysiologic and inotropic effects of O-benzyl-phosphocreatine in rabbit myocardium

L15 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Thermal properties, crystal lattice energy, mechanism and energetics of the thermal decomposition of hydrochlorides of 2-amino acid esters

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Anxiety alleviating compositions containing lower alkyl N-[amino(arylamino carbonyl)iminomethyl]-N-methylglycinates

L15 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Bromination of creatine, creatinine, and ethyl creatinate

L15 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Stimulating the central nervous system

L15 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI 3-Creatinyl-4-methyl-5-(2-hydroxyethyl)thiazolyl pyrophosphate

L15 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI 3-Creatinyl-4-methyl-5-(2-hydroxyethyl)thiazolyl pyrophosphate

=> d l15 2 ti fbib abs

L15 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
TI Creatine ester pronutrient compounds and formulations
AN 2002:220380 CAPLUS
DN 136:246810
TI Creatine ester pronutrient compounds and formulations
IN Vennerstrom, Jonathan L.; Miller, Donald W.
PA Board of Regents of the University of Nebraska, USA
SO PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2002022135 A1 20020321 WO 2001-US28788 20010914
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
 CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
 HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
 LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
 RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
 VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 US 2000-232969PP 20000914
 AU 2001090939 A5 20020326 AU 2001-90939 20010914
 US 2000-232969PP 20000914
 WO 2001-US28788W 20010914
 EP 1324760 A1 20030709 EP 2001-971000 20010914
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 US 2000-232969PP 20000914
 WO 2001-US28788W 20010914
 JP 2004508407 T2 20040318 JP 2002-526385 20010914
 US 2000-232969PP 20000914
 WO 2001-US28788W 20010914
 US 2003-365666 20030212
 US 2000-232969PP 20000914
 WO 2001-US28788A2 20010914
 NO 2003000937 A 20030424 NO 2003-937 20030228
 US 2000-232969PP 20000914
 WO 2001-US28788W 20010914
 US 2003-363761 20030305
 WO 2001-US28788W 20010914

AB The present invention describes a method for providing creatine to an
 animal which includes receiving a creatine ester by the animal. The
 creatine ester is suitable for being modified by the animal to form
 creatine.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	9.34	215.92

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.74	-4.42

FILE 'REGISTRY' ENTERED AT 10:04:19 ON 01 JUL 2004
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STRUCTURE FILE UPDATES: 30 JUN 2004 HIGHEST RN 701907-96-2
 DICTIONARY FILE UPDATES: 30 JUN 2004 HIGHEST RN 701907-96-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

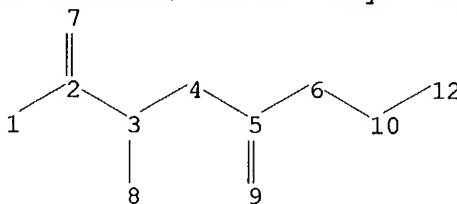
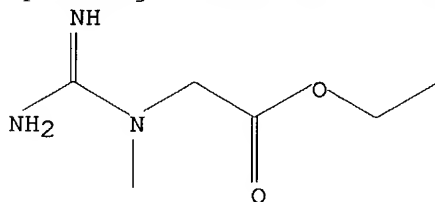
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e ethyl creatinate/cn

E1	1	ETHYL COUMARILATE/CN
E2	1	ETHYL COUMARINATE/CN
E3	0 -->	ETHYL CREATINATE/CN
E4	1	ETHYL CRESOL RED A/CN
E5	1	ETHYL CROTONATE/CN
E6	1	ETHYL CROTONATE-MALEIC ACID COPOLYMER/CN
E7	1	ETHYL CROTONOYLACETATE/CN
E8	1	ETHYL CROTYLIDENECYANOACETATE/CN
E9	1	ETHYL CRYSTAL VIOLET/CN
E10	1	ETHYL CYANACETATE/CN
E11	1	ETHYL CYANATE/CN
E12	1	ETHYL CYANIDE/CN

=>

Uploading C:\Examination Auxillary files\10647825\10647825 ethyl creatinate.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 12

chain bonds :

1-2 2-3 2-7 3-4 3-8 4-5 5-6 5-9 6-10 10-12

exact/norm bonds :

1-2 2-3 2-7 3-4 3-8 5-6 5-9 6-10

exact bonds :

4-5 10-12

Hydrogen count :

4:>= minimum 2 8:>= minimum 3

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

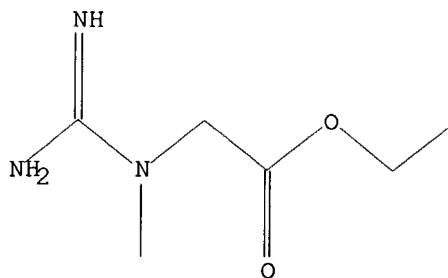
10:CLASS 12:CLASS

L16 STRUCTURE UPLOADED

=> d l16

L16 HAS NO ANSWERS

L16 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l16

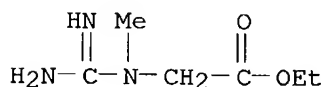
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:exact
 ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
 FULL SEARCH INITIATED 10:09:34 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 1 ANSWERS
 SEARCH TIME: 00.00.01

L17 1 SEA EXA FUL L16

=> d l17

L17 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 15366-29-7 REGISTRY
 CN Glycine, N-(aminoiminomethyl)-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Creatine, ethyl ester (6CI, 8CI)
 FS 3D CONCORD
 MF C6 H13 N3 O2
 CI COM
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, USPATFULL
 (*File contains numerically searchable property data)
 DT.CA Caplus document type: Journal; Patent
 RL.P Roles from patents: BIOL (Biological study); USES (Uses); NORL (No role in record)
 RL.NP Roles from non-patents: RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> search l17

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:end
 SEARCH ENDED BY USER

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
58.22	274.14

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-4.42

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FILE COVERS 1907 - 1 Jul 2004 VOL 141 ISS 1
FILE LAST UPDATED: 30 Jun 2004 (20040630/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l17

L18 4 L17

=> d l18 1-4 ti fbib abs

L18 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
TI Creatine ester pronutrient compounds and formulations
AN 2002:220380 CAPLUS
DN 136:246810
TI Creatine ester pronutrient compounds and formulations
IN Vennerstrom, Jonathan L.; Miller, Donald W.
PA Board of Regents of the University of Nebraska, USA
SO PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002022135	A1	20020321	WO 2001-US28788	20010914
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2000-232969PP 20000914				

AU 2001090939	A5	20020326	AU 2001-90939	20010914
			US 2000-232969PP	20000914
			WO 2001-US28788W	20010914
EP 1324760	A1	20030709	EP 2001-971000	20010914
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
			US 2000-232969PP	20000914
			WO 2001-US28788W	20010914
JP 2004508407	T2	20040318	JP 2002-526385	20010914
			US 2000-232969PP	20000914
			WO 2001-US28788W	20010914
US 2003212130	A1	20031113	US 2003-365666	20030212
			US 2000-232969PP	20000914
			WO 2001-US28788A2	20010914
NO 2003000937	A	20030424	NO 2003-937	20030228
			US 2000-232969PP	20000914
			WO 2001-US28788W	20010914
US 2003212136	A1	20031113	US 2003-363761	20030305
			WO 2001-US28788W	20010914

AB The present invention describes a method for providing creatine to an animal which includes receiving a creatine ester by the animal. The creatine ester is suitable for being modified by the animal to form creatine.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
TI Bromination of creatine, creatinine, and ethyl creatinate
AN 1967:473848 CAPLUS
DN 67:73848
TI Bromination of creatine, creatinine, and ethyl creatinate
AU Rudakova, I. P.; Pospelova, T. A.; Yurkevich, A. M.
CS Vses. Nauch.-Issled. Vitaminal. Inst., Moscow, USSR
SO Zhurnal Obshchei Khimii (1967), 37(2), 335-8
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Russian
AB Br (2.2 g.) added to 3 g. creatine in AcOH at 35-40° and heated 40 min. at 55-60° gave 44.9% creatine-HBr, m. 150-1° (EtOH-Et2O), identical with that formed from creatine and HBr. Creatinine and Br similarly gave 78.5% creatinine-HBr, decomposing at 225-6° (also formed with HBr), while creatine and HCl in dry EtOH gave 78% creatine Et ester HCl salt, m. 164-5° (EtOH-Et2O). N.M.R. spectra of the products, and ir spectrum of creatine-HBr were shown.

L18 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
TI 3-Creatinyl-4-methyl-5-(2-hydroxyethyl)thiazolyl pyrophosphate
AN 1958:82931 CAPLUS
DN 52:82931
OREF 52:14699f-h
TI 3-Creatinyl-4-methyl-5-(2-hydroxyethyl)thiazolyl pyrophosphate
IN Kominato, Kiyoshi
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
PI	JP 32009078	B4	19570000	JP	
GI	For diagram(s), see printed CA Issue.				
AB	Creatine (10 g.) in 100 ml. EtOH saturated with dry HCl gas, allowed to stand with cooling, and the product filtered off gave the Et ester (I) of creatine; this in 200 ml. AcOH treated dropwise with Br until Br color remained and kept overnight at 0° gave 13.5 g.				

H2NC(:NH)N(CH2CO2Et)CH2Br (II). II (10 g.) in 100 ml. EtOH-BuOH (1:1) treated dropwise with 10 g. H2NCSH below 30° formed H2NC(:NH)N(CH2CO2Et)CH2NHCSH (III) this treated dropwise with 38 g. AcCHClCH2CH2OH in 500 ml. EtOH below 60°, kept overnight, and the product concentrated in vacuo yielded 50% 3-creatinyl-4-methyl-5-(2-hydroxyethyl)thiazole (IV). IV (12 g.) in 100 ml. AcOH treated dropwise with POCl3, kept 4-5 days at 0°, the product heated with 60% EtOH containing a small amount of KOH, and cooled yielded 51% S.CH:NC1[CH2N(CH2CO2H)C(:NH)NH2].CMe:CCH2CH2OP(O)(OH)OP(O)(OH)2, m. 236-40°.

L18 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
 TI 3-Creatinyl-4-methyl-5-(2-hydroxyethyl)thiazolyl pyrophosphate
 AN 1958:82930 CAPLUS
 DN 52:82930
 OREF 52:14699e-f
 TI 3-Creatinyl-4-methyl-5-(2-hydroxyethyl)thiazolyl pyrophosphate
 IN Kominato, Kiyoshi
 DT Patent
 LA Unavailable
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 32009077	B4	19570000	JP	
AB	Creatine (100 g.) in 1 l. EtOH saturated with dry HCl gas, kept several hrs. at 0°, and the product filtered off gave Et ester (I) of creatine. I (100 g.) in 500 ml. AcOH and 100 g. red P, while cooling with ice, treated dropwise with 100 g. Br below 40°, then treated dropwise with 300 g. 4-methyl-5-(2-hydroxyethyl)thiazole, heated 1.5 hrs. at 55-60°, kept 10 days, the product filtered off, saponified with 60% EtOH containing a small amount of KOH, cooled with ice and salt, and the product filtered off gave 230 g. title compound, m. 238-40°.				

=>

Connection closed by remote host

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1	Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	"Ask CAS" for self-help around the clock
NEWS	3 May 10	PROUSDDR now available on STN
NEWS	4 May 19	PROUSDDR: One FREE connect hour, per account, in both May and June 2004
NEWS	5 May 12	EXTEND option available in structure searching
NEWS	6 May 12	Polymer links for the POLYLINK command completed in REGISTRY
NEWS	7 May 17	FRFULL now available on STN
NEWS	8 May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in Caplus

NEWS 9 May 27 CAplus super roles and document types searchable in REGISTRY
 NEWS 10 May 27 Explore APOLLIT with free connect time in June 2004
 NEWS 11 Jun 22 STN Patent Forums to be held July 19-22, 2004
 NEWS 12 Jun 28 Additional enzyme-catalyzed reactions added to CASREACT
 NEWS 13 Jun 28 ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG,
 and WATER from CSA now available on STN(R)

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
 NEWS HOURS STN Operating Hours Plus Help Desk Availability
 NEWS INTER General Internet Information
 NEWS LOGIN Welcome Banner and News Items
 NEWS PHONE Direct Dial and Telecommunication Network Access to STN
 NEWS WWW CAS World Wide Web Site (general information)

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:42:29 ON 01 JUL 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.63	0.63

FILE 'REGISTRY' ENTERED AT 11:44:07 ON 01 JUL 2004

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STRUCTURE FILE UPDATES: 30 JUN 2004 HIGHEST RN 701907-96-2

DICTIONARY FILE UPDATES: 30 JUN 2004 HIGHEST RN 701907-96-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e acetyl chloride/cn

E1	1	ACETYL CHAVICOL/CN
E2	1	ACETYL CHILIANOSIDE H/CN
E3	1 -->	ACETYL CHLORIDE/CN
E4	1	ACETYL CHLORIDE (O-NITROPHENYL)HYDRAZONE/CN
E5	1	ACETYL CHLORIDE 2-NITROPHENYLHYDRAZONE/CN

E6 1 ACETYL CHLORIDE 4-BROMO-2-NITROPHENYLHYDRAZONE/CN
 E7 1 ACETYL CHLORIDE 4-BROMOPHENYLHYDRAZONE/CN
 E8 1 ACETYL CHLORIDE CATION RADICAL/CN
 E9 1 ACETYL CHLORIDE, ((((((4-CHLOROPHENYL)METHYL)AMINO)IMINOMETHYL)AMINO)CARBONYL)AMINO)-, MONOHYDROCHLORIDE/CN
 E10 1 ACETYL CHLORIDE, ((((((4-CHLOROPHENYL)AMINO)IMINOMETHYL)AMINO)CARBONYL)AMINO)-, MONOHYDROCHLORIDE/CN
 E11 1 ACETYL CHLORIDE, ((((((CYCLOHEXYLMETHYL)AMINO)IMINOMETHYL)AMINO)CARBONYL)AMINO)-, MONOHYDROCHLORIDE/CN
 E12 1 ACETYL CHLORIDE, (((((ETHYLAMINO)IMINOMETHYL)AMINO)CARBONYL)AMINO)-, MONOHYDROCHLORIDE/CN

=> e3

L1 1 "ACETYL CHLORIDE"/CN

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.85	5.48

FILE 'CAPLUS' ENTERED AT 11:44:29 ON 01 JUL 2004

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FILE COVERS 1907 - 1 Jul 2004 VOL 141 ISS 1

FILE LAST UPDATED: 30 Jun 2004 (20040630/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l1

L2 8553 L1

=> esterification catalyst

91883 ESTERIFICATION

479 ESTERIFICATIONS

92007 ESTERIFICATION

(ESTERIFICATION OR ESTERIFICATIONS)

659365 CATALYST

663894 CATALYSTS

844913 CATALYST

(CATALYST OR CATALYSTS)

L3 7305 ESTERIFICATION CATALYST

(ESTERIFICATION (W) CATALYST)

=> l2(l)l3

L4 1 L2(L)L3

=> d l4 ti fbib abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Polyethylene glycol phase-transfer catalyzed synthesis of esters of
 carboxylic acids
 AN 1996:158956 CAPLUS
 DN 124:316667
 TI Polyethylene glycol phase-transfer catalyzed synthesis of esters of
 carboxylic acids
 AU Xie, Xiaojuan; Yang, Gaosheng; Yang, Fuguo; Song, Xueqing
 CS Dep. of Chem., Anhui Normal Univ., Wuhu, 241000, Peop. Rep. China
 SO Huaxue Yanjiu Yu Yingyong (1995), 7(4), 385-7
 CODEN: HYYIFM; ISSN: 1004-1656
 PB Huaxue Yanjiu Yu Yingyong Bianjibu
 DT Journal
 LA Chinese
 AB Acylation of alc. using polyethylene glycol as phase transfer catalyst has
 been studied. Eight esters of carboxylic acids can be obtained in good
 yields. The reaction of primary or secondary alcs. with acylations agents
 (Ac₂O, AcCl, or BzCl) is carried out by liquid-liquid PTC and tertiary alcs.
 with AcCl is carried out by solid-liquid PTC.

=> acyl halide

96154 ACYL
 240 ACYLS
 96257 ACYL
 (ACYL OR ACYLS)
 144680 HALIDE
 120062 HALIDES
 209654 HALIDE
 (HALIDE OR HALIDES)
 L5 2053 ACYL HALIDE
 (ACYL(W)HALIDE)

=> 13 and 15

L6 10 L3 AND L5

=> d 16 1-10 ti

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Two-step process for the preparation of alkyl 2-bromoalkanoates
 L6 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Method for preparation of O-acylated calixarenes
 L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Processes for preparation of 2-alkyl-2-adamantyl esters
 L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Catalytic, asymmetric α -halogenation
 L6 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Nucleophilic substitution at a trigonal carbon. Part 6. Substituent and
 bromide/chloride leaving group effects in the reactions of aromatic acyl
 chlorides with methanol in acetonitrile
 L6 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Preparation of aryl esters and an aromatic polyester by catalytic
 O-dealkylation and O-acylation of alkyl aryl ethers
 L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI A method of manufacturing esters of α -hydroxyalkanophenones as
 pharmaceutical and agrochemical intermediates

L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Esters of N-aroylaspartic acids and vinyl chloride polymers plasticized therewith

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Catalytic esterification by metal halides

L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Polyglycerol esters of aliphatic acids of relatively high molecular weight

=> d 16 1,2 ti fbib abs

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Two-step process for the preparation of alkyl 2-bromoalkanoates
 AN 2004:450601 CAPLUS
 TI Two-step process for the preparation of alkyl 2-bromoalkanoates
 IN Ruppin, Christophe; Magne, Vincent; Drivon, Gilles
 PA Atofina, Fr.
 SO Fr. Demande, 20 pp.
 CODEN: FRXXBL
 DT Patent
 LA French
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2847896	A1	20040604	FR 2002-15136	20021202
	WO 2004052818	A1	20040624	WO 2003-FR3505	20031127
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU				
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

FR 2002-15136 A 20021202

AB Alkyl 2-bromoalkanoates R1R2C(Br)CO2R3 [R1, R2 = H, (un)branched C1-10 alkyl; R3 = (un)branched C1-3 alkyl; e.g., Et 2-bromobutyrate] are prepared in two steps in which the first stage comprises the regioselective bromination of an alkanolic acid R1R2CHCO2H acid (e.g., butyric acid) with bromine in the presence of an **acyl halide** of the acid R1R2CHCOX (X = Cl, Br; e.g., butyryl chloride), then in one second stage the 2-bromoalkanoic acid R1R2C(Br)CO2H (e.g., 2-bromobutanoic acid) is esterified with an alc. R3OH (e.g., ethanol) in the presence of an acid **esterification catalyst** (e.g., sulfuric acid) with elimination from the reaction medium of the water of esterification by distillation using an alc. R3OH/2-bromoalkanoic acid molar ratio of 1.1-3. A production apparatus diagram is presented.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Method for preparation of O-acylated calixarenes
 AN 2002:235900 CAPLUS
 DN 136:279224
 TI Method for preparation of O-acylated calixarenes
 IN Yamanaka, Shunichiro; Sugata, Kazuaki
 PA Orient Chemical Industries, Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002088016	A2	20020327	JP 2000-272553 JP 2000-272553	20000908 20000908

OS CASREACT 136:279224; MARPAT 136:279224

AB O-acylated calixarenes or their derivs. are safely prepared in high yields at low cost without generating offensive odor. A process for preparation of O-acylated calixarenes or their derivs. comprises O-acylation of calixarenes or their derivs. using acid anhydrides or **acyl halides** in the presence of alkali and phase-transfer catalyst in an organic-water or organic-solid two phase system. The phase-transfer catalysts are polyoxyalkylene glycol diethers, quaternary ammonium salts, quaternary phosphonium salts, or cyclic poly ethers. This process does not use problematic reagents, e.g. pyridine presenting a problem of offensive odor in a scale up reaction, concentrated sulfuric acid undergoing exothermic reaction and presenting a danger for handling and a difficulty for controlling (cooling) the reaction system, and sodium hydride which is very reactive and undergo exothermic reactions accompanied by generation of hydrogen and foaming. Thus, tert-butylcalix[8]arene 2.0, polyoxyethylene glycol di-Et ether 0.25, and 50 weight% aqueous NaOH 9.0 g were added to 50 mL toluene, cooled at .apprx.10° with stirring, treated dropwise over 3 h with a solution of 3.25 g benzoyl chloride in 20 mL toluene at ≤20° under vigorous stirring, and stirred at 60° for 1 h to give 92.4% octabenzoyl-tert-butylcalix[8]arene.

=> d his

(FILE 'HOME' ENTERED AT 11:42:29 ON 01 JUL 2004)

FILE 'REGISTRY' ENTERED AT 11:44:07 ON 01 JUL 2004
E ACETYL CHLORIDE/CN

L1 1 E3

FILE 'CAPLUS' ENTERED AT 11:44:29 ON 01 JUL 2004

L2 8553 L1
L3 7305 ESTERIFICATION CATALYST
L4 1 L2(L)L3
L5 2053 ACYL HALIDE
L6 10 L3 AND L5

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	32.24	37.72
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.21	-2.21

FILE 'CAPLUS' ENTERED AT 12:01:57 ON 01 JUL 2004
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FILE COVERS 1907 - 1 Jul 2004 VOL 141 ISS 1
FILE LAST UPDATED: 30 Jun 2004 (20040630/ED)

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.46	38.18

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.21

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FILE 'REGISTRY' ENTERED AT 12:02:14 ON 01 JUL 2004
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JUN 2004 HIGHEST RN 701907-96-2
DICTIONARY FILE UPDATES: 30 JUN 2004 HIGHEST RN 701907-96-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

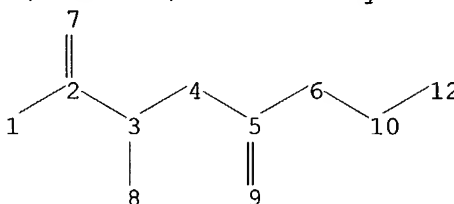
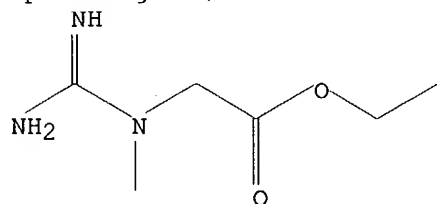
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Examination Auxillary files\10647825\10647825 ethyl creatinate.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 12

chain bonds :

1-2 2-3 2-7 3-4 3-8 4-5 5-6 5-9 6-10 10-12

exact/norm bonds :

1-2 2-3 2-7 3-4 3-8 5-6 5-9 6-10

exact bonds :
4-5 10-12

Hydrogen count :

4:>= minimum 2 8:>= minimum 3

Match level :

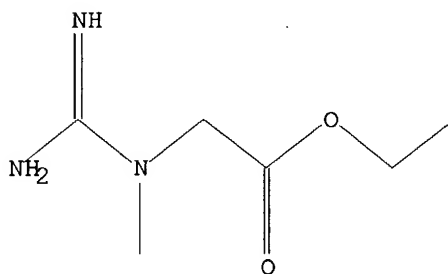
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 12:CLASS

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 17 sss sam

SAMPLE SEARCH INITIATED 12:03:01 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 8 TO 329

PROJECTED ANSWERS: 1 TO 80

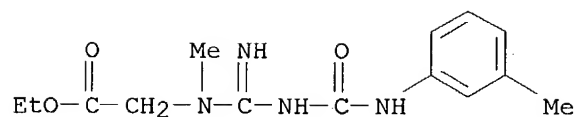
L8 1 SEA SSS SAM L7

=> d scan

L8 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Glycine, N-[imino[[[(3-methylphenyl)amino]carbonyl]amino]methyl]-N-methyl-
, ethyl ester, monohydrochloride (9CI)

MF C14 H20 N4 O3 . Cl H



● HCl

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
1.68	39.86

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.21

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 12:04:28 ON 01 JUL 2004